Cyclopentane

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.87

Global applicability domain: Inside

Local applicability domain index: 6.66e-01

Confidence level: 6.62e-01

Nearest Neighbors from the Training Set

Image not found
Cyclopentane
Measured: 3.00
Predicted: 2.87

Image not found
Cyclohexane
Measured: 3.44
Predicted: 3.48

Image not found
2-Methyl-2-butene
Measured: 2.67
Predicted: 2.67

Image not found
Cyclohexene
Measured: 2.86
Predicted: 2.90